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Asymptotic expansion of the Stark-Wannier states

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Abstract: In this article I give an iterative scheme to compute the coefficients of the power series expansion in the electric field parameter of the Stark-Wannier states in one-dimensional crystals. For symmetric crystals the asymptotic expansion up to the fourth order is explicitly computed, and for a solvable model the method is verified up to any order.

I. Introduction.

I consider the motion of an electron in a one-dimensional crystal under the action of an external uniform electric field of strength F. The Hamiltonian is of the form:

$$H_F = p^2 + V + Fx, \quad F > 0, \quad p = -i\frac{d}{dx}, \tag{I.1}$$

V is the potential of the crystal of period a. It is well known that, if the periodic potential is neglected, the electron is uniformly accelerated toward minus infinity. On the contrary, the study of the motion of an electron with Hamiltonian (I.1) is quite complicated, in fact when the electron is also submitted to a periodic potential, due to the crystal, it remains confined in a finite region for a large long time and, finally, will escape to infinity by tunnelling phenomena (see for instance Bentosela 1979 and Nenciu and Nenciu 1981). Hence, generically, we have for the electron metastable states, associated with ladders of resonances called Stark-Wannier states, but not actual bound states. However, if the crystal potential is sufficiently singular, as in the Krönig-Penney model, heuristic and numerical analysis (see Berezkowski and Ovchinnikov 1976 and Bentosela *et al* 1982) suggest that the electron cannot escape to infinity, so that in such a case we should have actual bound states.

From a rigorous point of view we have that, under some restrictions, the resonances exist (see the latest results in Bentosela and Grecchi 1990, Combes and Hislop 1990 and Grecchi *et al* 199: and Agler and Froese 1985 for the case of large electric field) although, for the general case, this is still an open problem. However, if resonances exist, they are exponentially close to the real axis for small electric field and well approximated by the ladders of eigenvalues of the single-band approximation (see Avron 1982, Bentosela *et al* 1982 and Buslaev and Dmitrieva 1990).

The single band approximation, going back to Wannier, leads to exact first order approximation (at least for symmetric potentials, where the Berry phase is absent). That is, H_F can be approximated up to a bounded term of order $O(F)$, by a direct sum of two Hamiltonians, where one of these has discrete point spectrum given by a ladder of eigenvalues (see Wannier 1960 and Avron *et al* 1977) In terms of spectral notions for H_F, such a ladder consists of a sequence of pseudo-eigenvalues for H_F and gives a spectral concentration for the absolutely continuous spectrum of H_F around its points (see Riddell 1967). In Nenciu and Nenciu 1981 (see also Nenciu 1991), by applying the Wannier single band approximation to H_F, where the bands are defined again so that the interband term between the first band and the others is of order F^{N+1}, N is an arbitrary positive integer the existence of pseudo-eigenvalues of any order is given. Moreover, in Nenciu and Nenciu 198: the same scheme works for the three-dimensional case where the electric field is parallel with a reciprocal lattice vector; an exponentially decay of the pseudo-eigenvectors along the electric field direction is also obtained.

Since the latest experimental results on the Stark-Wannier model (see for instance Voisin *et al* 1988, Voisin 1990a and 1990b and Soucal *et al* 1990 and 1991) it seems that an approximation of the Stark-Wannier states more accurate than the Wannier single-band approximation will be useful. In order to compute the asymptotic expansion of the pseudo-eigenvalues, coinciding with the asymptotic expansion of the resonances (if existent), in this article I use a "time-independent" version of the Nenciu-Nenciu method already seen in a previous paper (Grecchi *et al* 1990) and suggested also in Nenciu 1981 and Bentosela 1990. More precisely, in section II I obtain a sequence of Bloch operators H^N, having non-local periodic potential of integral type, such that the first gap is not empty and the interband term in H_F between the first band of H^N and the others is a bounded operator of order F^{N+1}. In particular, in the crystal momentum representation (CMR) H_F becomes $\tilde{H}_F = \mathbf{E}^N + F\mathbf{X}^N + iF\mathbf{D}$, where $\mathbf{E}^N$ and $\mathbf{X}^N$ can be computed by the following iterative scheme:

$$
\left\{
\begin{array}{lll}
\mathbf{U}^{j^+}\left(\mathbf{E}^j + F\mathbf{W}^j\right)\mathbf{U}^j & = & \mathbf{E}^{j+1}, \quad \text{where } \mathbf{E}^{j+1} \text{ is a diagonal matrix} \\
\mathbf{W}^j & := & \mathcal{P}_1\mathbf{X}^j\mathcal{P}_1^\perp + \mathcal{P}_1^\perp\mathbf{X}^j\mathcal{P}_1 \\
\mathbf{X}^{j+1} & := & i\mathbf{U}^{j^+}\frac{d\mathbf{U}^j}{dk} + \mathbf{U}^{j^+}(\mathbf{X}^j - \mathbf{W}^j)\mathbf{U}^j \;=\; \mathbf{X}^{j+1^+}, \quad j = 0,\, 1,\, \ldots\,,\, N.
\end{array}
\right.
\tag{I.2}
$$

Here, $\mathbf{E}^j$ is the diagonal matrix representing the Bloch operator H^j, $\mathbf{X}^j$ is the interband matrix, $\mathbf{W}^j$ is the interband matrix between the first band and the others, $\mathbf{U}^j$ is a unitary matrix, $\mathcal{P}_1$ is the projection on the first band and $\mathcal{P}_1^\perp = \mathbb{1} - \mathcal{P}_1$. Since the boundedness of the terms $\mathbf{W}^j$, the asymptotic expansion for the pseudo-eigenvalues follows by computing, at each step, the Rayleigh-Schrödinger series for $\mathbf{E}^j + F\mathbf{W}^j$.

In section III, I explicitly compute the asymptotic expansion for the pseudo-eigenvalues of H_F of fourth order in the case of symmetric crystals. By comparing this asymptotic expansion with the F complex one, already computed in Bentosela *et al* 1988, we have that the terms of second order are generically different. Hence, the existence of a horn of singularities tangent to the real axis for the eigenvalues of H_F, F complex, is suggested (see Grecchi *et al* 1990).

In section IV I verify up to any order the iterative scheme given in section II for an exactly solved model. In this model the periodic potential of H_F consists of a ladder of $\delta-$interactions with strength that goes to infinity. In such a case, we can de-couple H_F in a family of operators $\{H_{F,\ell}\}_{\ell\in\mathbb{Z}}$, where $H_{F,\ell}$ is formally defined by $p^2 + Fx$ with Dirichlet boundary conditions on $2\pi(\ell-1)$ and $2\pi\ell$. Hence, H_F has purely point spectrum and the Stark-Wannier states are actual bound states.

In Appendix I briefly resume the CMR, the representation of the position operator x in the CMR and some estimates about the band functions and the interband matrix useful in section II and III.

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II. Description of the iterative scheme and principal results.

Let us consider the Hamiltonian of the form

$$
H_F := H^0 + FX^0 \tag{II.1}
$$

where $H^0 := p^2 + V$, $X^0 = x$, $p = -i\frac{d}{dx}$ and $F > 0$. Here, V is a real potential which commutes with the translation operator T_a (we can assume, without loss of generality, $a = 2\pi$) and is infinitesimally relatively bounded with respect to p^2 in the form sense. Hence, periodic real-valued potentials $V(x)$ belonging to $L^2_{loc}(\mathsf{R})$ and real potentials defined in the form sense as the Krönig-Penney potential are both considered here. By KLMN Theorem (see Reed and Simon 1975 Theorem X.17) the operator H_F, formally defined in (II.1), is essentially self-adjoint on $C_0^\infty(\mathsf{R})$; let $\mathsf{D}(H_F)$ be its self-adjointness domain.

Let $\Sigma(H^0) = \bigcup_{n=1}^\infty [E_n^{b,0}, E_n^{t,0}]$ be the spectrum of the Bloch operator H^0. In the following we shall assume that the first gap $(E_1^{t,0}, E_2^{b,0})$ of H^0 is not empty, that is there exists $d_0 > 0$ such that $E_2^{b,0} - E_1^{t,0} > d_0$.

Now, as it has been announced in the Introduction, we give an iterative scheme such that, at the $N-$th step, the non-diagonal part in (II.1) between the first band and the others is of order F^{N+1}, N is an arbitrary positive integer. Hence, by applying the Wannier single-band approximation we obtain pseudo-eigenvalues for H_F. Since the interband term has expectation value zero on the associated pseudo-eigenvectors, the order of these pseudo-eigenvalues is F^{2N+1}.

In particular, we describe the iterative scheme at the first step and, by using induction hypothesis on N, at the generic step. Since the construction is essentially the same in both cases, in the second one we shall report as much as possible to the first one leaving out the details.

First step of the iterative scheme.

Let W^0 be the interband term in (II.1) between the first band and the others:

$$W^0 := -(1 - 2P_1^0)\left[P_1^0, X^0\right]_- = P_1^0 X^0 \left(\mathbb{1} - P_1^0\right) + \left(\mathbb{1} - P_1^0\right) X^0 P_1^0, \tag{II.2}$$

where P_1^0 is the spectral eigen-projection of H^0 corresponding to the first band $[E_1^{b,0}, E_1^{t,0}]$. We have that W^0 is bounded, because the first gap is open (see formula (A.24)), and is an integral operator with kernel $\mathcal{V}^0(x,y)$:

$$\left(W^0\psi\right)(x) := \int_{\mathsf{R}} \mathcal{V}^0(x,y)\psi(y)dy, \tag{II.3}$$

where (see Reed and Simon 1978, Theorem XIII.85 and problem XIII.134):

$$\begin{aligned}\mathcal{V}^0(x,y) &= \int_{\mathcal{B}}(x+y)e^{ik(x-y)}u_1^{k,0}(x)\overline{u_1^{k,0}(y)}dk + \\ &- 2\int_{\mathcal{B}}dk\int_{\mathcal{B}}dh\int_{\mathsf{R}}dz\left\{ze^{ik(x-z)}u_1^{k,0}(x)\overline{u_1^{k,0}(z)}e^{ih(z-y)}u_1^{h,0}(z)\overline{u_1^{h,0}(y)}\right\},\end{aligned} \tag{II.4}$$

$\psi_1^{k,0}(x) = e^{ikx}u_1^{k,0}(x)$ is the Bloch function of H^0 associated with $E_1^0(k)$, k belongs to the Brillouin zone $\mathcal{B} = (-1/2, +1/2]$. Hence W^0 is symmetric, $W^0 = W^{0^+}$, and commutes with the translation operator $T_{2\pi}$. In fact, one can verify that $\mathcal{V}^0(x,y) = \overline{\mathcal{V}^0(y,x)}$ and $\mathcal{V}^0(x+2\pi,y) = \mathcal{V}^0(x,y-2\pi)$. Therefore defining again the operator H_F on the same self-adjointness domain $\mathsf{D}(H_F)$ as

$$H_F := H^1 + FX^1, \tag{II.5}$$

where $X^1 \equiv X^1(F) := X^0 - W^0$ and $H^1 \equiv H^1(F) := H^0 + FW^0$, we have that H^1 is a symmetric Bloch operator, i.e.:

$$H^1 = H^{1^+} \quad \text{and} \quad \left[T_{2\pi}, H^1\right]_- = 0, \tag{II.6}$$

with periodic potential given by $V + FW^0$. From (II.6) and the boundedness of W^0 it follows that the spectrum of H^1 is given by bands and is stable with respect to the spectrum of H^0 as $F \to 0$. In particular, choosing $F \le F_1$, $F_1 := d_0/(4\|W^0\|)$, the first gap $(E_1^{t,1}, E_2^{b,1})$ of H^1 is still open, i.e. there exists $d_1 > 0$ such that $E_2^{b,1} - E_1^{t,1} > d_1$.

Now, in order to prove that the non-diagonal part in (II.5) between the first band of the Bloch operator H^1 and the others is a bounded operator of order F^2 we rewrite H_F in the CMR associated with the Bloch operator H^0 (see (A.13)-(A.14)):

$$\tilde{H}_F := \tilde{\mathcal{U}}^0 H_F(\tilde{\mathcal{U}}^0)^{-1} = \mathbf{E}^0 + F\mathbf{X}^0 + iF\mathbf{D}, \tag{II.7}$$

where $\tilde{\mathcal{U}}^0$ is the unitary transformation defined in (A.11) and (A.12) associated with the Bloch functions of H^0. Here, $\mathbf{E}^0 \equiv \mathbf{E}^0(k)$ is the diagonal matrix $(\mathbf{E}^0)_{n,m} = \delta_n^m E_n^0(k)$, $n, m \in \mathsf{N}$, where $E_n^0(k)$ are the band functions of H^0, $\mathbf{X}^0 \equiv \mathbf{X}^0(k)$ is the interband matrix and $\mathbf{D}$ is the derivative operator. Under this unitary transformation W^0 and H^1 become

$$\mathbf{W}^0 \equiv \mathbf{W}^0(k) := \tilde{\mathcal{U}}^0 W^0(\tilde{\mathcal{U}}^0)^{-1} = \mathcal{P}_1\mathbf{X}^0\mathcal{P}_1^\perp + \mathcal{P}_1^\perp\mathbf{X}^0\mathcal{P}_1, \tag{II.8}$$

where $\mathcal{P}_1^\perp = (\mathbb{1} - \mathcal{P}_1)$, $(\mathcal{P}_1 a)_n := \delta_1^n a_1$, $a = (a_n)_n \in \oplus_{n=1}^\infty L^2(\mathcal{B})$, and

$$\tilde{H}^1 := \tilde{\mathcal{U}}^0 H^1(\tilde{\mathcal{U}}^0)^{-1} = \mathbf{E}^0 + F\mathbf{W}^0. \tag{II.9}$$

Let $\mathbf{U}^0 \equiv \mathbf{U}^0(k;F)$ be the unitary matrix such that

$$\mathbf{U}^{0^+}\left(\mathbf{E}^0 + F\mathbf{W}^0\right)\mathbf{U}^0 = \mathbf{E}^1, \quad \left(\mathbf{E}^1\right)_{n,m} = \delta_n^m E_n^1, \tag{II.10}$$

where $E_n^1 \equiv E_n^1(k;F)$ are the band functions of the Bloch operator H^1, $n \in \mathbb{N}$. In particular, since $\chi_n^0 \equiv \chi_n^0(k) = \tilde{\mathcal{U}}^0\psi_n^{k,0}$ and $\chi_n^1 \equiv \chi_n^1(k;F) = \tilde{\mathcal{U}}^0\psi_n^{k,1}$ are the Bloch functions of H^0 and H^1 respectively in the CMR, we have

$$\left(\mathbf{U}^0\right)_{n,m} = \langle \chi_n^0, \chi_m^1 \rangle_{\ell^2} = (\chi_m^1)_n. \tag{II.11}$$

Now, since the interband term $\mathbf{W}^0$ is bounded we can compute the asymptotic expansion of the elements of $\mathbf{U}^0$ and $\mathbf{E}^1$ up to any order in F by regular perturbation theory applied to (II.9). In fact, for any $k \in \mathcal{B} - \{0, +1/2\}$, we have

$$E_n^1 \equiv E_n^1(k;F) = E_n^0(k) + F\frac{\langle \chi_n^0, \mathbf{W}^0\chi_n^1 \rangle}{\langle \chi_n^0, \chi_n^1 \rangle}, \tag{II.12}$$

where $\chi_n^1 = \dfrac{\tilde{P}_n^0\chi_n^0}{\|\tilde{P}_n^0\chi_n^0\|}$, and

$$\tilde{P}_n^0 \equiv \tilde{P}_n^0(k;F) := \frac{-1}{2\pi i}\oint_{\gamma_n^0}\left[\tilde{H}^1 - z\right]^{-1} dz, \tag{II.13}$$

$\gamma_n^0 \equiv \gamma_n^0(k)$ is a positively oriented circular contour around the unperturbed isolated eigenvalue $E_n^0(k)$. Hence, the Rayleigh-Schrödinger series gives the asymptotic expansion for E_n^1 and χ_n^1, as $F \to 0$, uniformly in n.

On the contrary, for $k = 0$ and $1/2$ the two eigenvalues $E_n^0(k)$ and $E_{n+1}^0(k)$, $n > 1$, can be too close. In such a case we apply the regular degenerate perturbation theory, with multiplicity at most 2, instead of the non-degenerate one to compute the asymptotic expansion of E_n^1 (see for instance Landau and Lifsits 1959).

However, in both cases we have

$$\begin{aligned}\tilde{P}_1^0 &= \frac{-1}{2\pi i}\oint_{\gamma_1^0}\left[\tilde{H}^1 - z\right]^{-1} dz \\ &= \frac{-1}{2\pi i}\oint_{\gamma_1^0}\left[\mathbf{E}^0 - z\right]^{-1} dz + \frac{F}{2\pi i}\oint_{\gamma_1^0}\left[\mathbf{E}^0 - z\right]^{-1}\left(1 + F\mathbf{W}^0\left[\mathbf{E}^0 - z\right]^{-1}\right)^{-1} dz \\ &= \frac{-1}{2\pi i}\oint_{\gamma_1^0}\left[\mathbf{E}^0 - z\right]^{-1} dz + O(F), \quad \text{as } F \to 0,\end{aligned} \tag{II.14}$$

since $\mathbf{W}^0$ is bounded. Therefore, from (II.11) we have $\left(\mathbf{U}^0\right)_{n,1} = \delta_1^n + O(F)$, as $F \to 0$, for any $k \in \mathcal{B}$ and $n \in \mathbb{N}$.

Under the unitary matrix $\mathbf{U}^0$ the operator (II.7) becomes the following (still denoted $\tilde{H}_F$):

$$\tilde{H}_F = \mathbf{U}^{0^+}\left(\mathbf{E}^0 + F\mathbf{X}^0 + iF\mathbf{D}\right)\mathbf{U}^0 = \mathbf{E}^1 + F\mathbf{X}^1 + iF\mathbf{D}, \tag{II.15}$$

where

$$\mathbf{X}^1 \equiv \mathbf{X}^1(k;F) := i\mathbf{U}^{0^+}\frac{d\mathbf{U}^0}{dk} + \mathbf{U}^{0^+}(\mathbf{X}^0 - \mathbf{W}^0)\mathbf{U}^0, \quad \mathbf{X}^1 = \mathbf{X}^{1^+}. \tag{II.16}$$

In particular, (II.15) corresponds to the operator (II.5) rewritten in the CMR (associated with the Bloch operator H^1), in fact $\mathbf{E}^1 \equiv \mathbf{E}^1(k;F) = \tilde{\mathcal{U}}^1 H^1 (\tilde{\mathcal{U}}^1)^{-1}$ is the diagonal matrix whose elements are the band functions of the Bloch operator H^1 and

$$\tilde{\mathcal{U}}^1 X^1 (\tilde{\mathcal{U}}^1)^{-1} = iF\mathbf{D} + F\left(i\mathbf{U}^{0^+}\frac{d\mathbf{U}^0}{dk} + \mathbf{U}^{0^+}\left(\mathbf{X}^0 - \mathbf{W}^0\right)\mathbf{U}^0\right) \tag{II.17}$$

as one can verify.

Let us stress that in (II.16) all the gaps of H^1 are implicitly assumed open. In fact, if the $n-$th gap is empty, for some $n > 1$, the interband term $(\mathbf{X}^1)_{n,n+1}(k)$ is singular for $k = 0$ (if n is even) or $k = 1/2$ (if n is odd). In such a case, the definition of the CMR associated with H^1 must be modified (see for instance Avron 1982 §2). However, in view of the crucial estimate (II.20) this is not important, so that we can continue in the construction of the iterative process defining formally $\mathbf{X}^1$ as in (II.16) without any discussion for the degenerate case.

Since the first gap of H^1 is open and W^0 is bounded, the interband term $W^1 \equiv W^1(F)$ in (II.5), between the first band and the others,

$$\begin{aligned} W^1 &:= P_1^1 X^1\left(\mathbb{1} - P_1^1\right) + \left(\mathbb{1} - P_1^1\right)X^1 P_1^1 \\ &= P_1^1 x\left(\mathbb{1} - P_1^1\right) + \left(\mathbb{1} - P_1^1\right)xP_1^1 - P_1^1 W^0\left(\mathbb{1} - P_1^1\right) - \left(\mathbb{1} - P_1^1\right)W^0 P_1^1 \end{aligned} \tag{II.18}$$

is bounded for any $F \leq F_1$. Here P_1^1 is the spectral eigen-projection of H^1 corresponding to the first band $[E_1^{b,1}, E_1^{t,1}]$, distant $d_1 > 0$ from the remainder of the spectrum and coincident with $[E_1^{b,0}, E_1^{t,0}]$ in the limit $F \to 0$. In particular, we have that $\|W^1\| = \|\mathbf{W}^1\| \leq c_1 F$, for some $c_1 < \infty$ and any $F \leq F_1$, where $\mathbf{W}^1 \equiv \mathbf{W}^1(k;F) := \tilde{\mathcal{U}}^1 W^1 (\tilde{\mathcal{U}}^1)^{-1}$. In fact,

$$\mathbf{W}^1 = \mathcal{P}_1 \mathbf{X}^1 \mathcal{P}_1^\perp + \mathcal{P}_1^\perp \mathbf{X}^1 \mathcal{P}_1 = O(F), \quad \text{as } F \to 0, \tag{II.19}$$

because $\left(\mathbf{U}^0\right)_{n,1} = \delta_1^n + O(F)$. That is, there exists $c_1 < \infty$ such that for any F, $F \leq F_1$, the following estimate holds:

$$\|\mathbf{W}^1\| = \left\{ \sum_{n=1}^{\infty} \int_{\mathcal{B}} |W_{n,1}^1|^2 dk \right\}^{1/2} \leq c_1 F, \quad \text{where } W_{n,1}^1 := \left(\mathbf{W}^1\right)_{n,1}. \tag{II.20}$$

The iterative scheme at any finite step.

By induction on N let us consider the operator

$$H_F := H^N + FX^N \tag{II.21}$$

self-adjoint on the domain $\mathsf{D}(H_F)$, where

$$H^N := H^0 + F\sum_{j=0}^{N-1} W^j \quad \text{and} \quad X^N := X^0 - F\sum_{j=0}^{N-1} W^j. \tag{II.22}$$

Here W^j is the interband term between the first band of the Bloch operator H^j and the others, $j = 0, 1, \ldots, N-1$; in particular, it is a bounded operator of integral type, symmetric and invariant with respect to the translation $T_{2\pi}$; moreover we have that $W^j = O(F^j)$, as $F \to 0$. Hence, H^N is a symmetric Bloch operator with the first gap not empty for any $F \leq F_N$, for some $F_N > 0$, i.e. $E_2^{b,N} - E_1^{t,N} > d_N$, $d_N > 0$.

Let W^N be the interband term in (II.21) between the first band and the others:

$$W^N := P_1^N X^N \left(\mathbb{1} - P_1^N\right) + \left(\mathbb{1} - P_1^N\right) X^N P_1^N, \tag{II.23}$$

where P_1^N is the spectral eigen-projection of H^N corresponding to the first band $[E_1^{b,N}, E_1^{t,N}]$, distant d_N from the remainder of the spectrum and coincident with $[E_1^{b,0}, E_1^{t,0}]$ in the limit $F \to 0$. Since $d_N > 0$ and by the boundedness of each W^j, W^N is bounded too. In particular, by induction on N we have $\|W^N\| \leq c_N F^N$ for some $c_N < \infty$ and any $F \leq F_N$. Besides, as in the $N = 0$ case, one quickly verifies that W^N is a symmetric operator of integral type and commutes with the translation operator $T_{2\pi}$.

Now, following the preceding construction we define again the operator H_F on the same self-adjointness domain $\mathsf{D}(H_F)$ as

$$H_F = H^{N+1} + FX^{N+1}, \tag{II.24}$$

where $X^{N+1} \equiv X^{N+1}(F) := X^N - W^N$ and $H^{N+1} \equiv H^{N+1}(F) := H^N + FW^N$. By the above cited properties on H^N and W^N it follows that H^{N+1} is a symmetric Bloch operator, i.e.

$$H^{N+1^+} = H^{N+1} \quad \text{and} \quad \left[H^{N+1}, T_{2\pi}\right]_- = 0, \tag{II.25}$$

and its spectrum is stable with respect to the spectrum of H^N. In particular, choosing $F \leq F_{N+1}$, $F_{N+1} := \min\left\{F_N, d_N/(4\|W^N\|)\right\}$, the first gap of H^{N+1} is still open, i.e. there exists $d_{N+1} > 0$ such that $E_2^{b,N+1} - E_1^{t,N+1} > d_{N+1}$.

Let

$$\tilde{H}_F := \tilde{\mathcal{U}}^N H_F (\tilde{\mathcal{U}}^N)^{-1} = \mathbf{E}^N + F\mathbf{X}^N + iF\mathbf{D} \tag{II.26}$$

and

$$\tilde{H}^{N+1} := \tilde{\mathcal{U}}^N H^{N+1} (\tilde{\mathcal{U}}^N)^{-1} = \mathbf{E}^N + F\mathbf{W}^N \tag{II.27}$$

be the CMR (associated with the Bloch operator H^N) of H_F and H^{N+1}, where $\mathbf{E}^N \equiv \mathbf{E}^N(k;F)$ is the diagonal matrix whose diagonal elements are the band functions of H^N, $\mathbf{X}^N \equiv \mathbf{X}^N(k;F)$ is the interband matrix and

$$\mathbf{W}^N \equiv \mathbf{W}^N(k;F) := \tilde{\mathcal{U}}^N W^N (\tilde{\mathcal{U}}^N)^{-1} = \mathcal{P}_1 \mathbf{X}^N \mathcal{P}_1^{\perp} + \mathcal{P}_1^{\perp} \mathbf{X}^N \mathcal{P}_1. \tag{II.28}$$

Let $\mathbf{U}^N \equiv \mathbf{U}^N(k;F)$ be the unitary matrix such that:

$$\mathbf{U}^{N^+} \left(\mathbf{E}^N + F\mathbf{W}^N\right) \mathbf{U}^N = \mathbf{E}^{N+1}, \quad \left(\mathbf{E}^{N+1}\right)_{n,m} = \delta_n^m E_n^{N+1}, \tag{II.29}$$

where $E_n^{N+1} \equiv E_n^{N+1}(k;F)$ are the band functions of the Bloch operator H^{N+1}, $n \in \mathbb{N}$.

Under this unitary transformation (II.26) becomes the following (still denoted $\tilde{H}_F$):

$$\tilde{H}_F = \mathbf{U}^{N^+} \left(\mathbf{E}^N + F\mathbf{X}^N + iF\mathbf{D}\right) \mathbf{U}^N = \mathbf{E}^{N+1} + F\mathbf{X}^{N+1} + iF\mathbf{D} \tag{II.30}$$

where

$$\mathbf{X}^{N+1} \equiv \mathbf{X}^{N+1}(k;F) := i\mathbf{U}^{N^+} \frac{d\mathbf{U}^N}{dk} + \mathbf{U}^{N^+}(\mathbf{X}^N - \mathbf{W}^N)\mathbf{U}^N, \quad \mathbf{X}^{N+1^+} = \mathbf{X}^{N+1}. \tag{II.31}$$

Now, by applying the regular non-degenerate perturbation theory as done in (II.14) we have that $\left(\mathbf{U}^N\right)_{n,1} = \delta_1^n + O(F^{N+1})$, as $F \to 0$, since $\mathbf{W}^N = O(F^N)$. Hence, we obtain the following estimate for the interband term in (II.30) between the first band and the others

$$\mathbf{W}^{N+1} = \mathcal{P}_1 \mathbf{X}^{N+1} \mathcal{P}_1^\perp + \mathcal{P}_1^\perp \mathbf{X}^{N+1} \mathcal{P}_1 = O(F^{N+1}), \quad \text{as } F \to 0. \tag{II.32}$$

In particular, there exists $c_{N+1} < \infty$ such that for any $F < F_{N+1}$

$$\|\mathbf{W}^{N+1}\| = \left\{ \sum_{n=1}^\infty \int_{\mathcal{B}} |W_{n,1}^{N+1}|^2 dk \right\}^{1/2} \leq c_{N+1} F^{N+1}, \quad \text{where } W_{n,1}^{N+1} := \left(\mathbf{W}^{N+1}\right)_{n,1}. \tag{II.33}$$

The above results can be summarized as follows:

Theorem 1. *Let $H^0 = p^2 + V$ be a Bloch operator with the first gap not empty, where V is a real potential invariant under the translation by 2π and infinitesimally relatively bounded with respect to p^2 in the form sense.*

Let $\tilde{H}_F$ be the CMR (associated with the Bloch operator H^0) of $H_F := H^0 + Fx$, $F > 0$,

$$\tilde{H}_F := \tilde{\mathcal{U}}^0 H_F (\tilde{\mathcal{U}}^0)^{-1} = \mathbf{E}^0 + F\mathbf{X}^0 + iF\mathbf{D}. \tag{II.34}$$

Then, for any positive integer N there exist $F_N > 0$ and a unitary matrix $\mathbf{V}^N \equiv \mathbf{V}^N(k;F)$ such that for any $F < F_N$

$$\mathbf{V}^{N^+} \tilde{H}_F \mathbf{V}^N = \mathbf{E}^N + F\mathbf{X}^N + iF\mathbf{D} \tag{II.35}$$

approaches, up to a bounded term of order F^{N+1} the Wannier de-coupled operator

$$\left(E_1^N + F(\mathbf{X}^N)_{1,1} + iF\frac{d}{dk} \right) \oplus \mathcal{P}_1^\perp \left(\mathbf{E}^N + F\mathbf{X}^N + iF\mathbf{D} \right) \mathcal{P}_1^\perp. \tag{II.36}$$

In particular, $\mathbf{V}^N$ is given by $\mathbf{V}^N := \mathbf{U}^0\mathbf{U}^1 \dots \mathbf{U}^{N-1}$, where $\mathbf{U}^j \equiv \mathbf{U}^j(k;F)$ are unitary matrices defined by the following iterative scheme

$$\left\{ \begin{array}{l} \mathbf{U}^{j^+} \left(\mathbf{E}^j + F\mathbf{W}^j \right) \mathbf{U}^j = \mathbf{E}^{j+1}, \quad \text{where } \mathbf{E}^{j+1} \text{ is a diagonal matrix} \\ \mathbf{W}^j := \mathcal{P}_1 \mathbf{X}^j \mathcal{P}_1^\perp + \mathcal{P}_1^\perp \mathbf{X}^j \mathcal{P}_1 \\ \mathbf{X}^{j+1} := i\mathbf{U}^{j^+} \dfrac{d\mathbf{U}^j}{dk} + \mathbf{U}^{j^+}(\mathbf{X}^j - \mathbf{W}^j)\mathbf{U}^j = \mathbf{X}^{j+1^+}, \quad j = 0, 1, \dots, N-1. \end{array} \right. \tag{II.37}$$

Remark 2. Following Avron *et al* 1977, the single band approximation of (II.35)

$$E_1^N + FX_{1,1}^N + iF\frac{d}{dk}, \qquad X_{1,1}^N := (\mathbf{X}^N)_{1,1}, \tag{II.38}$$

has discrete spectrum given by the ladder of non-degenerate eigenvalues

$$\lambda_{1,\ell}^N(F) = \langle E_1^N \rangle + F\langle X_{1,1}^N \rangle + 2\pi\ell F, \qquad \ell \in \mathbb{Z}, \tag{II.39}$$

where $\langle\cdot\rangle$ denotes the mean value on the Brillouin zone $\mathcal{B}$, with associated eigenvectors $f_{1,\ell}^N \in \oplus_{n=1}^\infty L^2(\mathcal{B})$:

$$\left[f_{1,\ell}^N(k;F)\right]_n = \delta_1^n \exp\left[-i/F\int^k \left(\lambda_{1,\ell}^N - E_1^N(h) - FX_{1,1}^N(h)\right)dh\right]. \tag{II.40}$$

Since the expectation value of $\mathbf{W}^N$ on the eigenvectors $f_{1,\ell}^N$ is zero, (II.39) represents a ladder of pseudo-eigenvalues of H_F of order $2N+1$ (see Riddell 1967, especially Lemma 3.2 and formula (15)). A similar result is also given in the paper of Nenciu and Nenciu 1982, see Theorems 2 and 3 and related remarks.

Remark 3. The convergence of the iterative process as $N \to \infty$ has not been proved. Hence, in general, we haven't bound states. However, for singular potential, as the Krönig-Penney potential, we believe that the above iterative process can be proved to be convergent as $N \to \infty$ as suggested by the model shown in Section IV.

III. Asymptotic expansion of the pseudo-eigenvalues.

Theorem 1 gives the existence of pseudo-eigenvalues of H_F of arbitrary order in F as pointed out in Remark 2. Moreover, by using the iterative scheme (II.37) and the regular perturbation theory one can compute the asymptotic expansion of these pseudo-eigenvalues. Now we are going to compute the asymptotic expansion of the pseudo-eigenvalues of H_F of fourth order.

Choosing $N=2$ in Theorem 1 and Remark 2 it follows that

$$\lambda_{1,\ell}^2(F) = \langle E_1^2 \rangle + 2\pi\ell F + F\langle X_{1,1}^2 \rangle, \quad \ell \in \mathbb{Z}, \tag{III.1}$$

is a ladder of pseudo-eigenvalues of H_F of fourth order.

For sake of simplicity we shall assume all the gaps of H^0 open and V an even local potential, i.e. $V(x) = V(-x)$. Hence, $X_{n,m}^0 = -X_{m,n}^0$ and $X_{n,n}^0 = 0$ for any k (see Appendix).

From (II.37) we have that:

$$X^2_{1,1} := \left(i\mathbf{U}^{1^+}\frac{d\mathbf{U}^1}{dk}\right)_{1,1} + \left(\mathbf{U}^{1^+}(\mathbf{X}^1 - \mathbf{W}^1)\mathbf{U}^1\right)_{1,1} = O(F^4), \quad \text{as } F \to 0. \tag{III.2}$$

In fact

$$\begin{aligned}\left(\mathbf{U}^{1^+}(\mathbf{X}^1 - \mathbf{W}^1)\mathbf{U}^1\right)_{1,1} &= \sum_{n,m\neq 1} \left(\mathbf{U}^{1^+}\right)_{1,n} X^1_{n,m}\mathbf{U}^1{}_{m,1} \\ &= \sum_{n,m\neq 1} \overline{\mathbf{U}^1}_{n,1} X^1_{n,m}\mathbf{U}^1{}_{m,1} = O(F^4),\end{aligned} \tag{III.3}$$

because $\left(\mathbf{U}^1\right)_{n,1} = \delta^n_1 + O(F^2)$, and a simple calculation gives

$$\left(\mathbf{U}^{1^+}\frac{d\mathbf{U}^1}{dk}\right)_{1,1} = \frac{1}{\|\tilde{P}^1_1\chi^1_1\|}\left\langle \tilde{P}^1_1\chi^1_1, \frac{d(\tilde{P}^1_1\chi^1_1)}{dk}\right\rangle = O(F^4), \tag{III.4}$$

where

$$\tilde{P}^1_1\chi^1_1 = \chi^1_1 + F\sum_{n\neq 1}\frac{X^1_{n,1}}{E^1_1 - E^1_n}\chi^1_n + O(F^4). \tag{III.5}$$

Hence, (III.1) becomes

$$\lambda^2_{1,\ell}(F) = \langle E^2_1\rangle + 2\pi\ell F + O(F^5) \quad \text{as } F \to 0. \tag{III.6}$$

Now, from the Rayleigh-Schrödinger series for E^2_1 and E^1_1 (see for instance Reed and Simon IV, Chapter XII §1), we obtain

$$\begin{aligned}\lambda^2_{1,\ell}(F) &= \langle E^1_1\rangle + 2\pi\ell F + F\langle X^1_{1,1}\rangle - F^2\sum_{m\neq 1}\left\langle\frac{|X^1_{m,1}|^2}{E^1_m - E^1_1}\right\rangle + O(F^5) \\ &= \langle E^0_1\rangle + 2\pi\ell F - F^2\sum_{m\neq 1}\left\langle\frac{|X^0_{m,1}|^2}{E^0_m - E^0_1}\right\rangle + F\langle X^1_{1,1}\rangle + \\ &\quad - F^2\sum_{m\neq 1}\left\langle\frac{|X^1_{m,1}|^2}{E^1_m - E^1_1}\right\rangle - 2F^4\sum_{n,m\neq 1}\left\langle\frac{|X^0_{n,1}|^2|X^0_{m,1}|^2}{(E^0_n - E^0_1)^2(E^0_m - E^0_1)}\right\rangle + O(F^5).\end{aligned} \tag{III.7}$$

Finally, by using again (II.37) to compute $X^1_{1,1}$ up to the fourth order and $X^1_{m,1}$ up to the second order we have the above mentionated asymptotic expansion of the pseudo-eigenvalues of H_F of fourth order as $F \to 0$:

$$\lambda_{1,\ell}^2 = \langle E_1^0\rangle + 2\pi\ell F - F^2 \sum_{m\neq 1}\left\langle \frac{|X_{m,1}^0|^2}{E_m^0 - E_1^0}\right\rangle - 2F^4 \sum_{n,m\neq 1}\left\langle \frac{|X_{n,1}^0|^2|X_{m,1}^0|^2}{(E_n^0 - E_1^0)^2(E_m^0 - E_1^0)}\right\rangle +$$
$$- F^4 \sum_{m\neq 1}\left\langle \frac{\left| i\frac{d}{dk}\left(\frac{X_{m,1}^0}{E_m^0 - E_1^0}\right) + \sum_{r\neq 1}\frac{X_{m,r}^0 X_{r,1}^0}{E_r^0 - E_1^0}\right|^2}{E_m^0 - E_1^0}\right\rangle + O(F^5). \tag{III.8}$$

In fact

$$\begin{aligned} X_{m,1}^1 &:= i\left(\mathrm{U}^{0+}\frac{d\mathrm{U}^0}{dk}\right)_{m,1} + \left(\mathrm{U}^{0+}(\mathrm{X}^0 - \mathrm{W}^0)\mathrm{U}^0\right)_{m,1} \\ &= \frac{i}{\|\tilde P_1^0\chi_1^0\|}\left\langle \tilde P_m^0\chi_m^0, \frac{d(\tilde P_1^0\chi_1^0)}{dk}\right\rangle + \sum_{r,s\neq 1}\frac{\langle \tilde P_m^0\chi_m^0,\chi_r^0\rangle}{\|\tilde P_m^0\chi_m^0\|}X_{r,s}^0\frac{\langle \chi_s^0, \tilde P_1^0\chi_1^0\rangle}{\|\tilde P_1^0\chi_1^0\|} \\ &= -iF\frac{d}{dk}\left(\frac{X_{m,1}^0}{E_m^0 - E_1^0}\right) - F\sum_{r\neq 1}\frac{X_{m,r}^0 X_{r,1}^0}{E_r^0 - E_1^0} + O(F^2), \end{aligned} \tag{III.9}$$

and

$$\begin{aligned} X_{1,1}^1 &:= i\left(\mathrm{U}^{0+}\frac{d\mathrm{U}^0}{dk}\right)_{1,1} + \left(\mathrm{U}^{0+}(\mathrm{X}^0 - \mathrm{W}^0)\mathrm{U}^0\right)_{1,1} \\ &= F^2\sum_{r,s\neq 1}\frac{X_{1,r}^0 X_{r,s}^0 X_{s,1}^0}{(E_r^0 - E_1^0)(E_s^0 - E_1^0)} + \frac{F^2}{2}\sum_{n\neq 1}\frac{d}{dk}\left[\frac{X_{n,1}^0}{E_n^0 - E_1^0}\right]^2 + O(F^4) \\ &= \frac{F^2}{2}\sum_{n\neq 1}\frac{d}{dk}\left[\frac{X_{n,1}^0}{E_n^0 - E_1^0}\right]^2 + O(F^4), \end{aligned} \tag{III.10}$$

because $X_{r,s}^0 = -X_{s,r}^0$, and so $\langle X_{1,1}^1\rangle = O(F^4)$ since the interband terms and the band functions are periodic on $\mathcal{B}$.

Remark 4. By comparing the asymptotic expansion (III.5) of the pseudo-eigenvalues of H_F with the asymptotic expansion of the eigenvalues $\lambda_{1,\ell}(F)$ of H_F for F complex, with $\Im F > 0$ and $|\arg F - \pi/2| < \delta$, $\delta < \pi/2$ (see Bentosela *et al* 1988), we have that the second order terms are, generically, different. In particular, as pointed out in Grecchi *et al* 1990, this would be a further support to the existence of a horn of singularities, tangent to the real axis in the origin, for $\lambda_{1,\ell}(F)$.

IV. An exactly solvable model with pure point spectrum.

In this section we present a model whose spectral problem is exactly solved by using the iterative scheme, slightly modified, given in Section II. In particular, in such a model the iterative scheme reproduces the same results given by the regular perturbation theory applied to the family of de-coupled operators $\{H_{F,\ell}\}_{\ell\in Z}$ as F goes to zero.

Let

$$H^0 = p^2 + V_\alpha, \quad \text{where } V_\alpha := \sum_{\ell=-\infty}^{+\infty} \alpha \cdot \delta(x - 2\ell\pi), \; -\infty < \alpha \le +\infty, \tag{IV.1}$$

be the Krönig-Penney Hamiltonian (see Albeverio *et al* 1988 for a review, especially Chapter III.2). It is well known that H^0 has, for $0 < \alpha < +\infty$, absolutely continuous spectrum given by bands $[E^b_{n,\alpha}, E^t_{n,\alpha}]$, $E^t_{n,\alpha} = n^2/4$.

On the contrary, for $\alpha = +\infty$, H^0 has purely point spectrum given by the eigenvalues $E_{n,\infty}$ with infinite multiplicity. In particular, for any $k \in \mathcal{B}$, we have that

$$E_{n,\infty}(k) \equiv E_n = n^2/4 \tag{IV.2}$$

with associated Bloch function

$$\psi^k_{n,\infty} \equiv \psi^k_n = e^{ikx} u^k_n(x), \tag{IV.3}$$

where $u^k_n(x)$ are periodic functions, with period 2π, given by

$$u^k_n(x) = \sqrt{2}\sin(nx/2)e^{-ikx} \cdot \begin{cases} 1 & \text{if } -\pi < x \le 0 \\ (-1)^n e^{i2\pi k} & \text{if } 0 \le x < +\pi \end{cases} \tag{IV.4}$$

Now, $H_F = H^0 + Fx$ in the CMR (associated with the Bloch operator H^0) becomes $\tilde{H}_F = \mathbf{E}^0 + F\mathbf{X}^0 + iF\mathbf{D}$ where $\mathbf{E}^0$ is the diagonal matrix whose elements are the $k-$independent band functions and the elements of the interband matrix $\mathbf{X}^0$ are given by

$$(\mathbf{X}^0)_{n,m} \equiv X^0_{n,m} = i\int_0^{2\pi} \overline{u^k_n(x)} \cdot \frac{\partial u^k_m(x)}{\partial k} \frac{dx}{2\pi} \tag{IV.5}$$

and they are $k-$independent too. In particular, from (IV.4) we have that

$$\begin{cases} X^0_{n,n} = -\pi & \\ X^0_{n,m} = 0 & \text{if } n \ne m \text{ and } n+m \text{ is even} \\ X^0_{n,m} = -\frac{16}{\pi}\left[\frac{nm}{(m^2-n^2)^2}\right] & \text{if } n+m \text{ is odd}. \end{cases} \tag{IV.6}$$

Hence, $\mathbf{X}^0 = \mathbf{X}^{0+}$ and it is bounded.

Now, let $\mathbf{U}^0$ be the $k-$independent unitary matrix such that:

$$\mathbf{U}^{0^+}\left(\mathbf{E}^0 + F\mathbf{X}^0\right)\mathbf{U}^0 = \mathbf{E}^1, \quad \mathbf{E}^1 \text{ is diagonal}. \tag{IV.7}$$

Under the unitary matrix $\mathbf{U}^0$, $\tilde{H}_F$ becomes the following (still denoted $\tilde{H}_F$)

$$\tilde{H}_F = \mathbf{U}^{0^+}\tilde{H}_F\mathbf{U}^0 = \mathbf{E}^1 + iF\mathbf{D}. \tag{IV.8}$$

Hence, the interband matrix vanishes and so H_F has purely point spectrum given by the sequence of ladders of eigenvalues $\lambda_{n,\ell}(F) = E_n^1 + 2\pi\ell F$, $n \in \mathbb{N}$ and $\ell \in \mathbb{Z}$, where E_n^1 is the n–th eigenvalue of $\mathbf{E}^0 + F\mathbf{X}^0$. In particular, by the Rayleigh-Schrödinger series we can obtain the convergent expansion of these eigenvalues, that is we have

$$\lambda_{n,\ell}(F) = \frac{n^2}{4} + (2\ell - 1)\pi F - F^2\frac{1024}{\pi^2}\sum_{m:m+n \text{ is odd}}\frac{n^2m^2}{(m^2-n^2)^5} + O(F^3), \quad \text{as } F \to 0. \tag{IV.9}$$

Let us stress that the spectral problem for H_F can be solved in the following way too. Since a δ–interaction with infinite strength consists of a Dirichlet boundary condition on the point supporting the δ–interaction, we can de-couple H_F as $H_F = \oplus_{\ell=-\infty}^{+\infty} H_{F,\ell}$, where the operator $H_{F,\ell}$ is formally defined by $p^2 + Fx$ with Dirichlet boundary conditions on $2\pi(\ell - 1)$ and $2\pi\ell$. Hence H_F has purely point spectrum given by

$$\Sigma(H_F) = \cup_{\ell\in\mathbb{Z}}\Sigma(H_{F,\ell}) = \Sigma(H_{F,0}) \oplus \{2\pi\ell F\}_{\ell\in\mathbb{Z}}. \tag{IV.10}$$

Let

$$\frac{d^2\psi}{dx^2} - Fx\psi = \lambda\psi, \quad \psi(-2\pi) = \psi(0) = 0, \tag{IV.11}$$

be the spectral problem for $H_{F,0}$. Taking $y = -F^{-2/3}(\lambda - Fx)$ (IV.11) becomes

$$\frac{d^2\psi}{dy^2} - y\psi = 0, \quad \psi(-F^{-2/3}(\lambda + 2\pi F)) = \psi(-F^{-2/3}\lambda) = 0. \tag{IV.12}$$

Here, choosing ψ of the form $\psi(y) = c_1 Ai(y) + c_2 Bi(y)$, where Ai and Bi are the Airy functions, the Dirichlet boundary condition (IV.12) implies that c_1 and c_2 must be the non-zero solutions of the following linear system

$$\begin{cases} c_1 \cos\theta\left(F^{-2/3}(\lambda + 2\pi F)\right) + c_2 \sin\theta\left(F^{-2/3}(\lambda + 2\pi F)\right) = 0 \\ c_1 \cos\theta(F^{-2/3}\lambda) + c_2 \sin\theta(F^{-2/3}\lambda) = 0, \end{cases} \tag{IV.13}$$

where θ is defined by $Ai(-x) = M(x)\cos\theta(x)$ and $Bi(-x) = M(x)\sin\theta(x)$ (see Abramowitz and Stegun 1972, [10.4.69]). Hence we obtain the following condition on λ:

$$\theta\left(F^{-2/3}(\lambda+2\pi F)\right) - \theta(F^{-2/3}\lambda) = -n\pi, \quad n = 1,2,\dots . \tag{IV.14}$$

Now, from the asymptotic expansion of $\theta(x)$ for x large (see Abramowitz and Stegun 1972, [10.4.79]), i.e. for F small, we obtain the following asymptotic expansion for λ_n:

$$\lambda_n(F) = n^2/4 - F\pi + F^2\left(\frac{\pi^2}{3n^2} - \frac{5}{n^4}\right) + O(F^3) \quad \text{as } F \to 0 \tag{IV.15}$$

in agreement with (IV.9).

Appendix. On the one-dimensional CMR.

Let us consider the Bloch Hamiltonian of the form

$$H_B = p^2 + V, \quad p = -i\frac{d}{dx} \tag{A.1}$$

where V is a real potential and invariant with respect to the translation $x \to x+a$. Moreover, it is assumed infinitesimally relatively bounded with respect to p^2 in the form sense. Hence, by the KLMN Theorem (Reed and Simon 1975 Theorem X.17), there exists an unique self-adjoint operator, still denoted H_B, having the same form domain of p^2 and such that

$$\langle\phi, H_B\psi\rangle = \langle\phi, p^2\psi\rangle + \langle\phi, V\psi\rangle, \quad \forall\psi,\phi \in C_0^\infty(\mathrm{R}) \tag{A.2}$$

Such a class of potentials includes the following ones:

a) periodic real-valued potentials $V(x)$ belonging to $L^2_{loc}(\mathrm{R})$ (see for instance Reed and Simon 1978, Theorem XIII.96);

b) non-local potentials of integral type with kernel $\mathcal{V}(x,y) \in L^2(\mathrm{R}^2)$:

$$(V\psi)(x) := \int_{\mathrm{R}} \mathcal{V}(x,y)\psi(y)dy \tag{A.3}$$

symmetric, $V = V^+$, and invariant with respect to the translation $x \to x+a$, that is $\mathcal{V}(x,y) = \overline{\mathcal{V}(y,x)}$ and $\mathcal{V}(x+a,y) = \mathcal{V}(x,y-a)$.

c) Krönig-Penney potential, i.e. $V = \sum_{j\in\mathrm{Z}} \alpha\cdot\delta(x-ja)$ where α is real and $\delta(x)$ is the Dirac delta function supported on 0 (see for instance Reed and Simon 1975 p.168);

In the following, for sake of simplicity, we shall assume $a = 2\pi$ and V positive, that is $\langle V\psi, \psi\rangle \geq 0$.

Let $\mathcal{B} = (-1/2, +1/2]$ be the Brillouin zone. It is well known that, for each $k \in \mathcal{B}$, the operator formally defined by H_B on $L^2\left([0, 2\pi], \frac{dx}{2\pi}\right)$ with the boundary conditions

$$\psi^k(2\pi) = e^{ik2\pi}u^k(0) \quad \text{and} \quad \frac{d\psi^k}{dx}(2\pi) = e^{ik2\pi}\frac{du^k}{dx}(0), \tag{A.4}$$

has compact resolvent. Hence, for any $k \in \mathcal{B}$, we have a complete set of orthonormal eigenfunctions $\psi_n^k(x)$ on $L^2([0, 2\pi]\frac{dx}{2\pi})$, $n \in \mathsf{N}$, called Bloch functions:

$$H_B\psi_n^k(x) = E_n(k)\psi_n^k(x) \tag{A.5}$$

and the discrete spectrum consists of a sequence of eigenvalues

$$0 \leq E_1(k) \leq E_2(k) \leq \ldots \leq E_n(k) \leq \ldots, \quad \text{where } E_n(k) = (n+k)^2 + O\left(\frac{1}{n}\right) \quad \text{as } n \to \infty. \tag{A.6}$$

These eigenvalues, as functions of k, are called band functions and consist of branches which are analytic except possibly at point of degeneracy; degeneracy occurs, at most, for $k = 0$ or $1/2$. Moreover, they are even functions, $E_n(-k) = E_n(k)$, and periodic, $E_n(k+1) = E_n(k)$.

Let

$$E_n^t = \max_{k\in\mathcal{B}} E_n(k) \quad \text{and} \quad E_n^b = \min_{k\in\mathcal{B}} E_n(k), \tag{A.7}$$

then $\Sigma(H_B) = \bigcup_{n=1}^{\infty}[E_n^b, E_n^t]$; the closed interval $[E_n^b, E_n^t]$ is called n−th band and the open intervals $(-\infty, E_1^b)$ and (E_n^t, E_{n+1}^b) are called the 0−th and the n−th gap respectively.

Let us stress that the above properties are, usually, proved for local potential. However, they can be easily extended to the class of potentials considered here.

Now, by using the boundary conditions (A.4) we extend the eigenfunctions $\psi_n^k(x)$ on the whole real axis as $\psi_n^k(x) = e^{ikx}u_n^k(x)$, where $u_n^k(x)$ is a periodic function of period 2π. The Fourier coefficients $\omega_n^k(K)$, $K \in \mathsf{Z}$, of the periodic function $u_n^k(x)$:

$$u_n^k(x) = \sum_{K\in\mathsf{Z}} \omega_n^k(K)e^{iKx}. \tag{A.8}$$

are called momentum eigenfunctions and they are orthonormalized functions in the Hilbert space $\int_{\mathcal{B}}^{\oplus} \mathcal{H}'(k)\, dk$, $\mathcal{H}'(k) = \ell^2(\mathsf{Z})$. In terms of the momentum eigenfunctions the spectral problem for H_B becomes

$$(K+k)^2\omega_n^k(K)+\sum_{J\in Z}V_{J,K}\omega_n^k(J) = E_n(k)\omega_n^k(K), \quad k\in\mathcal{B} \text{ and } K\in Z, \tag{A.9}$$

where, for potentials of type *a)* $V_{J,K}=\tilde{V}_{K-J}$ is k-independent and coincides with the $(K-J)$-th Fourier coefficient of $V(x)$ and for potentials of type *b)* we have

$$V_{J,K}\equiv V_{J,K}(k) := \frac{1}{2\pi}\int_R dy\int_0^{2\pi}dx\left\{\mathcal{V}(x,x+y)e^{i(J+k)y}e^{-i(K-J)x}\right\}, \tag{A.10}$$

where $\overline{V_{J,K}} = V_{K,J}$ because $V=V^+$.

Now, we are going to define the Crystal Momentum Representation associated with the orthonormal complete set of the momentum eigenfunctions $\{\omega_n^k(K)\}_{n\in N}$ in $\int_{\mathcal{B}}^{\oplus}\mathcal{H}'(k)\,dk$. To this end, we shall assume all the gaps open, that is there is no degeneracy point on the real axis for any band function $E_n(k)$.

Let $\tilde{\mathcal{U}}$ be the unitary transformation:

$$\begin{aligned}\tilde{\mathcal{U}} &: L^2(R)\to\oplus_{n=1}^{\infty}L^2(\mathcal{B}) \quad \text{defined by:}\\ \psi &\to \left(\tilde{\mathcal{U}}\psi\right)_n(k) = a_n(k),\end{aligned} \tag{A.11}$$

where

$$\begin{aligned}a_n(k) &:= \left\langle\omega_n^k,\hat{\psi}(k)\right\rangle_{\ell^2}\\ &= \sum_{K\in Z}\overline{\omega_n^k(K)}\cdot\hat{\psi}(k,K);\end{aligned} \tag{A.12}$$

this is called the Crystal Momentum Representation of ψ. Here $\hat{\psi}(k,K):=\hat{\psi}(p)$, $p=k+K$, is the Fourier transform of ψ.

In this representation H_B and x become:

$$\begin{aligned}H_B &\to \tilde{\mathcal{U}}H_B\tilde{\mathcal{U}}^{-1} = \tilde{H}_B\\ x &\to \tilde{\mathcal{U}}x\tilde{\mathcal{U}}^{-1} = i\mathrm{D}+\mathrm{X}\end{aligned} \tag{A.13}$$

where, on the generic vector $a=(a_n)_n\in\oplus_{n=1}^{\infty}L^2(\mathcal{B})$ such that $a_n\in C^1(\mathcal{B})$ for each n, and only a finite number of a_n is not identically zero, act as:

$$\begin{aligned}\left(\tilde{H}_B a\right)_n(k) &= E_n(k)\cdot a_n(k),\\ (\mathbf{X}a)_n(k) &= \sum_{m=1}^{\infty} X_{n,m}(k)\cdot a_m(k), \qquad (A.14)\\ (\mathbf{D}a)_n(k) &= \frac{da_n(k)}{dk}.\end{aligned}$$

where

$$X_{n,m}(k) := i\left\langle \omega_n^k, \frac{d\omega_m^k}{dk}\right\rangle_{\ell^2} = i\int_0^{2\pi} \overline{u_n^k(x)}\cdot\frac{\partial u_m^k(x)}{\partial k}\frac{dx}{2\pi}, \qquad (A.15)$$

hence $\mathbf{X} = \mathbf{X}^+$. In particular, if V is an even local potential, i.e. $V(x) = V(-x)$, then the momentum eigenfunctions can be chosen real and such that $\omega_n^{-k}(-K) = \pm\omega_n^k(K)$. Hence, $X_{n,m}(k)$ has real part zero, so $X_{n,m}(k) = -X_{m,n}(k)$ and $X_{n,n} \equiv 0$, and $X_{n,m}(-k) = \pm X_{n,m}(k)$.

Now, differentiating with respect to k both sides of (A.9) and projecting them on the m–th momentum eigenfunction, we obtain:

$$2\langle\omega_m^k, \mathbf{K}(k)\omega_n^k\rangle + (E_m - E_n)\left\langle\omega_m^k, \frac{d\omega_n^k}{dk}\right\rangle + \mathsf{V}_{m,n} = \frac{dE_n(k)}{dk}\delta_n^m \qquad (A.16)$$

where

$$\left(\mathbf{K}(k)\omega_n^k\right)(K) := (K+k)\cdot\omega_n^k(K). \qquad (A.17)$$

Here

$$\begin{aligned}\mathsf{V}_{m,n} &:= i\sum_{J,K\in\mathsf{Z}}\int_{\mathsf{R}} dy\int_0^{2\pi}\frac{dx}{2\pi}\left\{y\mathcal{V}(x,x+y)e^{i(J+k)y}e^{-i(K-J)x}\omega_n^k(J)\overline{\omega_m^k(K)}\right\}\\ &= i\int_{\mathsf{R}} dy\int_0^{2\pi}\frac{dx}{2\pi}\left\{(y-x)\mathcal{V}(x,y)\overline{\psi_m^k(x)}\psi_n^k(y)\right\}\end{aligned} \qquad (A.18)$$

for potential of type *b)*. For a local potential $V(x)$ of type *a)* we have that $\mathsf{V}_{n,m} \equiv 0$ and the following formulas hold:

$$\left|\frac{dE_n(k)}{dk}\right| = 2|\langle\omega_n^k, \mathbf{K}(k)\omega_n^k\rangle| \qquad (A.19)$$

and

$$X_{n,m}(k) = 2i\frac{\langle\omega_n^k, \mathbf{K}(k)\omega_m^k\rangle}{E_m(k) - E_n(k)} \quad \text{if } n\neq m. \qquad (A.20)$$

Therefore, since

$$||\mathbf{K}(k)\omega_m^k||_{\ell^2} \leq \sqrt{E_m(k)}, \tag{A.21}$$

we have that

$$\left|\frac{dE_n(k)}{dk}\right| \leq 2\sqrt{E_n(k)} \quad \text{and} \quad |X_{n,m}(k)| \leq 2\frac{\sqrt{E_l(k)}}{|E_m(k)-E_n(k)|}, \; l := \min(n,m). \tag{A.22}$$

Thus, the interband term $\mathbf{W}$ between the $m-$th band and the others is bounded. In fact, choosing $m = 1$ for instance, we have

$$\mathbf{W} := \mathcal{P}_1\mathbf{X}\mathcal{P}_1^\perp + \mathcal{P}_1^\perp\mathbf{X}\mathcal{P}_1, \tag{A.23}$$

and

$$||\mathbf{W}||^2 = \sum_{n\neq 1}\int_{\mathcal{B}}|X_{n,1}|^2 dk \leq 4\sum_{n\neq 1}\frac{E_1^t}{|E_n^b - E_1^t|^2} < +\infty, \tag{A.24}$$

because $|E_n^b - E_1^t|^2 \sim n^4$ for n large enough (a more accurate estimate is given in Grecchi *et al* 1989).

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